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METHOD OF SOLUTION FOR VARIATIONAL PRINCIPLE USING BICUBIC HERMITE POLYNOMIAL

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In solving mixed boundary and initial value problems of a second order partial differential equation using spline functions, the computation may be simplified considerably if the variable in time can be truncated into arbitrary sections. Each section may have several node points for the spline functions in the time domain. This is true because we found from a previous paper[1] that the initial value problem can be solved in one direction using variational principle and

(CONT'D ON REVERSE)

20. ABSTRACT (CONT'D)

cubic Hermite Polynomials, without worrying about the conditions at the other end.

The end conditions of the adjoint system can be adjusted according to the end conditions of the original system so that the bilinear concomitant is identically zero. This satisfies the variational principle. A bilinear form of the original and adjoint variables is employed in determining the coefficients of the variations of the functions and their first derivatives. There is no term involving the variations of any higher derivatives. A bicubic Hermite Polynomial spline function is used which gives continuity in the function and first partial derivatives in space or time, together with the mixed first partial derivative in space and time. Algorithm and procedure of computation are given.

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INTRODUCTION

This report is concerned with the use of variational principles to solve a mixed boundary and initial value problem. From a previous paper[1] we understand that the far end conditions are not imposed for solutions in an initial value problem. This implies that the boundary value problem can be solved in strips of arbitrarily chosen intervals of time. The size of the computation can be reduced substantially if the time interval taken is sufficiently large and number of strips small. This depends, of course, on the accuracy of the method.

A procedure can be obtained for a recursive relationship in the time domain, where the final conditions of first strip can be regarded as initial conditions of the second strip. These recursive solutions can be obtained by using variational principles with the aid of the bicubic Hermite polynomial spline functions as finite elements.

ESTIMATION

A dynamical system can be modeled by the following partial differential equation.

$$L(\zeta)\ y_a(\zeta) = -Q(\zeta) \tag{1}$$

with appropriate boundary and initial conditions. In the above equation L is a linear operator, in both spatial and temporal domain, y_a is the dependent variable, Q is a forcing function and ζ represents all independent variables,

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[1] Shen, C. N. and Wu, J. J., "A New Variational Method for Initial Value Problems Using Piecewise Hermite Polynomial Spline Functions," presented at the 1981 Army Numerical Analysis and Computer Conference, Huntsville, AL, February 1981.

both spatial and temporal.

The inner product < > of an adjoint forcing function $\bar{Q}$ and the solution ($y_a(\zeta)$) of Eq. (1) can be used for the purpose of estimation. This inner product is

$$G[y_a] = \langle \bar{Q} y_a \rangle \tag{2}$$

The estimate y, which differs from the actual solution y_a of Eq. (1) by an increment

$$\delta y = y - y_a \quad , \tag{3}$$

then becomes

$$\begin{aligned} G[y] &= G[y_a + \delta y] \\ &= \langle \bar{Q}, (y_a + \delta y) \rangle \\ &= G[y_a] + \langle \bar{Q}, \delta y \rangle \end{aligned} \tag{4}$$

which is in error to first order in δy and $\bar{Q}$. This is undesirable because the error depends on the variation δy which is supposed to be arbitrary. Thus the estimate will not be accurate.

THE VARIATIONAL PRINCIPLE

A more accurate estimate can be made by constructing a variational principle[1] for Eq. (2). By using the adjoint variable $\bar{y}$ as a Lagrange multiplier for Eq. (1) added to G[y] we have

$$\begin{aligned} J[y,\bar{y}] &= G[y] + \langle \bar{y}, (Q + Ly) \rangle \\ &= \langle \bar{Q}, y \rangle + \langle \bar{y}, Q \rangle + \langle \bar{y}, Ly \rangle \end{aligned} \tag{5}$$

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[1]Shen, C. N. and Wu, J. J., "A New Variational Method for Initial Value Problems Using Piecewise Hermite Polynomial Spline Functions," presented at the 1981 Army Numerical Analysis and Computer Conference, Huntsville, AL, February 1981.

In order that J be a variational principle for G the following requirements must be satisfied.

(a) J is stationary about the function y_s which satisfies the relation in Eq. (1).

$$Ly_s = -Q \tag{6}$$

(b) The stationary value of J deduced from Eqs. (2) through (5) is

$$J[\bar{y},y] = G[y_s] + G[y_a] \tag{7}$$

Consider first the stationarity of J by taking the variation of Eq. (5)

$$\begin{aligned} \delta J &= \langle \bar{Q},\delta y\rangle + \langle \delta\bar{y},Q\rangle + \langle \delta\bar{y},Ly\rangle + \langle \bar{y},L\delta y\rangle \\ &= \langle \delta\bar{y},(Ly+Q)\rangle + \langle \delta y,(\overline{Ly}+\bar{Q})\rangle \\ &\qquad - \langle \delta y,\overline{Ly}\rangle + \langle \bar{y},L\delta y\rangle \end{aligned} \tag{8}$$

We will make an effort later to impose certain conditions in order that the following equality holds:

$$\langle \bar{y},L\delta y\rangle = \langle \delta y,\overline{Ly}\rangle \tag{9}$$

where $\bar{L}$ is the adjoint operator.

By combining Eqs. (8) and (9) one obtains

$$\delta J = \langle \delta\bar{y},(Ly+Q)\rangle + \langle \delta y,(\overline{Ly}+\bar{Q})\rangle = 0 \tag{10}$$

Since the variations $\delta\bar{y}$ and δy are arbitrary it leads to the requirement that the stationary values y_s and $\bar{y}_s$ must satisfy

$$Ly_s = -Q \tag{11}$$

$$\overline{Ly}_s = -\bar{Q} \tag{12}$$

Equation (11) is the same as Eq. (6), therefore J is stationary about the function y_s.

Equation (12) is the adjoint equation in terms of the adjoint operator $\bar{L}$, the adjoint variable $\bar{y}$, and the adjoint forcing function $\bar{Q}$.

It is noted that δJ in Eq. (10) vanishes and is independent of the arbitrary variations δy and $\delta \bar{y}$, in contrast with Eq. (4), where δG is in error to the first order in δy. By using δJ instead of δG one can claim that the estimate is more accurate and free from the arbitrary variations.

Using the relationship in Eq. (11) the stationary value of J from Eq. (5) is

$$J[\bar{y}_s, y_s] = \langle \bar{Q}, y_s \rangle + \langle \bar{y}_s, Q \rangle + \langle \bar{y}_s, L y_s \rangle = G[y_s] \qquad (13)$$

Since J is stationary and $\delta J \to 0$, then

$$G[y_s] \to G[y_a] \qquad (14)$$

which is the requirement given in Eq. (7).

It is noted that Eq. (10) contains no boundary terms to be satisfied. This bears an important point in the future discussion.

BILINEAR CONCOMITANT

We will find out the conditions for the assumed equality in Eq. (9) to be true. Let us consider the following bilinear concomitant:[2]

$$D = \langle \bar{y}, Ly \rangle - \langle y, \bar{L}\bar{y} \rangle \qquad (15)$$

The above expression can be integrated in two different ways and can also be written in terms of boundary conditions and initial conditions. It is assumed that these boundary conditions are assigned in such a manner that the

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[2]Stacey, W. M., Jr, Variational Methods in Nuclear Reactor Physics, Academic Press, 1974.

above bilinear concomitant is identically zero for all independent variables, i.e.,

$$D \equiv 0 \tag{16}$$

Then the first variations of D also vanish.

$$\delta D = \delta D(\delta\bar{y}) + \delta D(\delta y) = 0 \tag{17}$$

Since $\delta\bar{y}$ and δy are independent of each other, then

$$\delta D(\delta\bar{y}) = \langle \delta\bar{y}, Ly \rangle - \langle y, \bar{L}\delta\bar{y} \rangle = 0 \tag{18}$$

$$\delta D(\delta y) = \langle \bar{y}, L\delta y \rangle - \langle \delta y, \bar{L}\bar{y} \rangle = 0 \tag{19}$$

Equation (19) is identical to Eq. (9), which is the assumed equality previously. The implication is that if Eq. (16) is true then Eq. (9) or (19) is automatically true.

Since Eq. (15) can be expressed in terms of some integrals involving boundary conditions, Eq. (16) can be true if these boundary conditions are satisfied. The next section will discuss integral of bilinear expression and its boundary conditions.

INTEGRAL OF BILINEAR EXPRESSION

The integral of a bilinear expression for a two-dimensional second order problem in space-time can be written as

$$I = \int_{x_o}^{x_b} \int_{t_o}^{t_b} \psi[y(x,t),\bar{y}(x,t)]\,dt\,dx \tag{20}$$

where $\psi[y,\bar{y}]$ is a given bilinear expression in the form

$$\psi[y,\bar{y}] = \alpha y_t \bar{y}_t + \beta y_t \bar{y} + \gamma y \bar{y}_t + \ell y_x \bar{y}_x + \mu y_x \bar{y} + \nu y \bar{y}_x + \varepsilon y \bar{y} \tag{21}$$

The subscripts t and x indicate the partial derivatives of the function y and $\bar{y}$.

Equation (20) can be integrated by parts. Two different forms of integration and end conditions can be obtained. The first form of the integral is

$$I = -\int_{x_o}^{x_b}\int_{t_o}^{t_b} \bar{y}Ly\,dt\,dx + \int_{x_o}^{x_b} (\alpha y_t+\gamma y)\bar{y}\Big|_{t_o}^{t_b} dx + \int_{t_o}^{t_b} (\ell y_x+\nu y)\bar{y}\Big|_{x_o}^{x_b} dt \tag{22}$$

which is obtained by integrating by parts on the adjoint variable. On the other hand, we can perform integration on the original variables to give

$$I = -\int_{x_o}^{x_b}\int_{t_o}^{t_b} y\bar{L}\bar{y}\,dt\,dx + \int_{x_o}^{x_b} (\alpha \bar{y}_t+\beta \bar{y})y\Big|_{t_o}^{t_b} dx + \int_{t_o}^{t_b} (\ell \bar{y}_x+\mu \bar{y})y\Big|_{x_o}^{x_b} dt \tag{23}$$

where

$$Ly = (\alpha y_t)_t - \beta y_t + (\gamma y)_t + (\ell y_x)_x - \mu y_x + (\nu y)_x - \varepsilon y \tag{24}$$

and

$$\bar{L}\bar{y} = (\alpha \bar{y}_t)_t + (\beta \bar{y})_t - \gamma \bar{y}_t + (\ell \bar{y}_x)_x + (\mu \bar{y})_x - \nu \bar{y}_x - \varepsilon \bar{y} \tag{25}$$

For a two-dimensional second order system in space-time domain, Eq. (15) becomes

$$D = \int_{x_o}^{x_b}\int_{t_o}^{t_b} \bar{y}Ly\,dt\,dx - \int_{x_o}^{x_b}\int_{t_o}^{t_b} y\bar{L}\bar{y}\,dt\,dx \tag{26}$$

By equating Eqs. (22) and (23) and solving for D in Eq. (26), we are converting the double integral into two simple integrals in terms of the boundary conditions.

We can express the quantity D as the sum of two parts D_1 and D_2 as

$$D = D_1 + D_2$$

The terms in D_1 involve the initial conditions of y and $\bar{y}$ as

$$D_1 = \int_{x_o}^{x_b} \{\alpha_b(y_{tb}\bar{y}_b - \bar{y}_{tb}y_b) - \alpha_o(y_{to}\bar{y}_o - \bar{y}_{to}y_o)$$

$$+ (\gamma_b - \beta_b)y_b\bar{y}_b - (\gamma_o - \beta_o)y_o\bar{y}_o\}dx \tag{27}$$

The terms in D_2 involve the boundary conditions of y and $\bar{y}$ as

$$D_2 = \int_{t_o}^{t_b} \{\ell_b(y_{xb}\bar{y}_b - \bar{y}_{xb}y_b) - \ell_o(y_{xo}\bar{y}_o - \bar{y}_{xo}y_o)$$

$$+ (\nu_b - \mu_b)y_b\bar{y}_b - (\nu_o - \mu_o)y_o\bar{y}_o\}dt \tag{28}$$

In order that $D \equiv 0$ in Eq. (16), it requires that

$$D_1 \equiv 0 \tag{29a}$$

and

$$D_2 \equiv 0 \tag{29b}$$

END CONDITIONS FOR THE ADJOINT SYSTEMS

We may take four different cases in discussing the end conditions for the adjoint systems in order to satisfy the requirements in Eqs. (29a) and (29b)

(a). The Wave Equation: In this case Eq. (24) becomes

$$Ly = (\alpha y_t)_t + (\ell y_x)_x = 0 \tag{30}$$

and the coefficients are

$$\gamma_b = \beta_b, \quad \gamma_o = \beta_o, \quad \nu_b = \mu_b, \quad \nu_o = \mu_o$$

$$\alpha_b \neq 0, \ \alpha_o \neq 0, \ \ell_b \neq 0, \text{ and } \ell_o \neq 0 \tag{31}$$

Let us assume that the adjoint variables are

$$\bar{y}_b = ky_o, \quad \bar{y}_o = ky_b \tag{32}$$

$$\bar{y}_{tb} = -\alpha_b^{-1}\alpha_o ky_{to}, \quad \bar{y}_{to} = -\alpha_o^{-1}\alpha_b ky_{tb} \tag{33}$$

$$\bar{y}_{xb} = -\ell_b^{-1}\ell_o ky_{xo} \quad \text{and} \quad \bar{y}_{xo} = -\ell_o^{-1}\ell_b ky_{xb} \tag{34}$$

where k is constant.

The above boundary values satisfy the requirement that $D_1 = D_2 = 0$ in Eqs. (27) and (28). Thus it also satisfies Eq. (16) that

$$D \equiv 0$$

(b). Heat Equation: In this case Eq. (24) is

$$Ly = -\beta y_t + (\gamma y)_t + (\ell y_x)_x = 0 \tag{35}$$

and the coefficients are

$$\nu_b = \mu_b, \quad \nu_o = \mu_o, \quad \alpha_b = 0, \quad \alpha_o = 0$$

$$\gamma_b \neq \beta_b, \quad \gamma_o \neq \beta_o, \quad \ell_b \neq 0, \quad \ell_o \neq 0 \tag{36}$$

Let the adjoint variables be

$$\bar{y}_b = (\gamma_o-\beta_o)ky_o, \quad \bar{y}_o = (\gamma_b-\beta_b)ky_b \tag{37}$$

$$\bar{y}_{xb} = -\ell_b^{-1}\ell_o(\gamma_b-\beta_b)ky_{xo}, \quad \bar{y}_{xo} = -\ell_o^{-1}\ell_b(\gamma_o-\beta_o)ky_{xb} \tag{38}$$

We also have $D_1 = D_2 = 0$ and $D \equiv 0$.

(c). First order partials of x in Eq. (24) are missing, i.e.,

$$\nu_b = \mu_b, \quad \nu_o = \mu_o, \quad \gamma_b \neq \beta_b, \quad \gamma_o \neq \beta_o \tag{39}$$

Let

$$\bar{y}_b = (\gamma_o-\beta_o)ky_o, \quad \bar{y}_o = (\gamma_b-\beta_b)ky_o \tag{40}$$

$$\bar{y}_{tb} = -\alpha_b^{-1}\alpha_o(\gamma_b-\beta_b)ky_{to}, \quad \bar{y}_{to} = -\alpha_o^{-1}\alpha_b(\gamma_o-\beta_o)ky_{tb} \tag{41}$$

$$\bar{y}_{xb} = -\ell_b^{-1}\ell_o(\gamma_b-\beta_b)ky_{xo}, \quad \bar{y}_{xo} = -\ell_o^{-1}\ell_b(\gamma_o-\beta_o)ky_{xb} \tag{42}$$

We also have $D_1 = D_2 = 0$ and $D \equiv 0$.

(d). First order partials of t in Eq. (24) are missing.

$$\gamma_b = \beta_b, \quad \gamma_o = \beta_o, \quad \nu_b \neq \mu_b, \quad \nu_o \neq \mu_o$$

$$\alpha_b \neq 0, \quad \alpha_o \neq 0, \quad \ell_b \neq 0, \text{ and } \ell_o \neq 0 \tag{43}$$

Let

$$\bar{y}_b = (\nu_o-\mu_o)ky_o, \quad \bar{y}_o = (\nu_b-\mu_b)ky_b \tag{44}$$

$$\bar{y}_{tb} = -\alpha_b^{-1}\alpha_o(\nu_b-\mu_b)ky_{to}, \quad \bar{y}_{to} = -\alpha_o^{-1}\alpha_b(\nu_o-\mu_o)ky_{tb} \tag{45}$$

$$\bar{y}_{xb} = -\ell_b^{-1}\ell_o(\nu_b-\mu_b)ky_{xo}, \quad \bar{y}_{xo} = -\ell_o^{-1}\ell_b(\nu_o-\mu_o)ky_{xb} \tag{46}$$

We also have $D_1 = D_2 = 0$, and $D \equiv 0$.

From the expression $D \equiv 0$ in Eq. (15) we can conclude that $\delta D = 0$ in Eq. (19) and Eq. (9) hold, which leads to the condition in Eq. (10) that

$$\delta J = 0$$

for all arbitrary variations $\delta\bar{y}$ and δy.

FIRST VARIATION

Since the variations $\delta\bar{y}$ and δy are independent of each other, the part of δJ in Eq. (10) with variation $\delta\bar{y}$ can be expressed as

$$\delta J(\delta\bar{y}) = \int_{x_o}^{x_b}\int_{t_o}^{t_b} \delta\bar{y}Lydtdx + \int_{x_o}^{x_b}\int_{t_o}^{t_b} \delta\bar{y}Qdtdx = 0 \tag{47}$$

where Ly is given in Eq. (24) and contains second order partial differentials in y. It is intended to include only first order partial differentials and the function y itself in $\delta J(\delta\bar{y})$. This can be achieved by considering the variation of the bilinear expression I in Eqs. (20) and (21) which gives

$$\delta I = \delta I(\delta\bar{y}) + \delta I(\delta y) \tag{48}$$

where

$$\delta I(\delta\bar{y}) = \int_{x_o}^{x_b} \int_{t_o}^{t_b} [(\alpha y_t+\gamma y)\delta\bar{y}_t + (\beta y_t+\varepsilon y+\mu y_x)\delta\bar{y} + (\ell y_x+\nu y)\delta\bar{y}_x]dtdx \quad (49)$$

A different version of the above variation can be obtained from Eq. (22) as

$$\delta I(\delta\bar{y}) = -\int_{x_o}^{x_b} \delta\bar{y}Lydtdx + \int_{x_o}^{x_b} \delta y(\alpha y_t+\gamma y)\Big|_{t_o}^{t_b} dx + \int_{t_o}^{t_b} \delta\bar{y}(\ell y_x+\nu y)\Big|_{x_o}^{x_b} dt \quad (50)$$

Equating Eqs. (49) and (50), solving for the term containing integral for $\delta\bar{y}Ly$ and substituting into Eq. (47) we have

$$\delta J(\delta\bar{y}) = \int_{x_o}^{x_b} (\alpha y_t+\gamma y)\delta\bar{y}\Big|_{t_o}^{t_b} dx + \int_{t_o}^{t_b} (\ell y_x+\nu y)\delta\bar{y}\Big|_{x_o}^{x_b} dt + \int_{x_o}^{x_b} \int_{t_o}^{t_b} \delta\bar{y}Qdtdx - \int_{x_o}^{x_b} \int_{t_o}^{t_b} [\alpha y_t+\gamma y)\delta\bar{y}_t + (\beta y_t+\varepsilon y+\mu y_x)\delta\bar{y} + (\ell y_x+\nu y)\delta\bar{y}_x]dtdx = 0 \quad (51)$$

This is the key equation which uses variational principle in solving a mixed initial and boundary value problem. The above equation contains only δy, δy_t, and δy_x and none of the variations of higher derivatives. The dependent variable contains only y, y_t, and y_x and no higher partials.

TRANSFORMATION OF COORDINATES

The integral signs in Eq. (51) can be converted into summation signs if discrete intervals for integration are used. We may take some scale factors to nondimensionalize the problem by giving

$$t_o = 0,\ t_b = 1 \qquad 0 \leqslant t \leqslant 1 \tag{52}$$

$$x_o = 0,\ x_b = 1 \qquad 0 \leqslant x \leqslant 1 \tag{53}$$

Moreover, Eq. (51) can be discretized by letting

$$\xi = Ht - i+1 \qquad 0 \leqslant \xi \leqslant 1 \qquad i = 1,2,\ldots,H \tag{54}$$

$$\eta = Kx - j+1 \qquad 0 \leqslant \eta \leqslant 1 \qquad j = 1,2,\ldots,K \tag{55}$$

where H and K are number of intervals for t and x respectively.

Thus the partial derivatives are

$$y_t = \frac{\partial y}{\partial t} = H \frac{\partial y}{\partial \xi} = Hy_\xi \tag{56}$$

$$y_x = \frac{\partial y}{\partial x} = K \frac{\partial y}{\partial \eta} = Ky_\eta \tag{57}$$

Use of Eqs. (52) through Eq. (57) then leads to

$$\begin{aligned}
\delta \bar{J}(\delta y) = & \sum_{j=1}^{K} \int_0^1 [\alpha H y_\xi(i,j) + \gamma y(i,j)]\,\delta\bar{y}(i,j)\Big|_{t_o}^{t_b} \frac{1}{K}\, d\eta \\
& + \sum_{i=1}^{H} \int_0^1 [\ell K y_\eta(i,j) + \nu y(i,j)]\,\delta\bar{y}(i,j)\Big|_{x_o}^{x_b} \frac{1}{H}\, d\xi \\
& + \sum_{j=1}^{K} \int_0^1 \{\sum_{i=1}^{H} \int_0^1 \delta\bar{y}(i,j)Q\, \frac{1}{H}\, d\xi\}\, \frac{1}{K}\, d\eta \\
& - \sum_{j=1}^{K} \int_0^1 \{\sum_{i=1}^{H} \int_0^1 [(\alpha H y_\xi(i,j) + \gamma y(i,j))H\delta\bar{y}_\xi(i,j) \\
& + (\beta H y_\xi(i,j) + \varepsilon y(i,j) + \mu K y_\eta(i,j))\,\delta\bar{y}(i,j) \\
& + (\ell K y_\eta(i,j) + \nu y(i,j))K\delta\bar{y}_\eta(i,j)]\, \frac{1}{H}\, d\xi\}\, \frac{1}{H}\, d\eta
\end{aligned} \tag{58}$$

GRID SYSTEMS

The (16x1) vector $Y^{(i,j)}$ has a grid of four (4x1) vectors $Y_1^{(i,j)}$ through $Y_4^{(i,j)}$, thus

$$Y^{(i,j)} = \{[Y_1^{(i,j)}]^T\ [Y_2^{(i,j)}]^T\ [Y_3^{(i,j)}]^T\ [Y_4^{(i,j)}]^T \tag{59}$$

Each of the (4x1) vectors has four components, consisting of the function, its first partials in both directions, and its mixed partial.

$$Y_1^{(i,j)} = \begin{bmatrix} y(\xi_i,\eta_j) \\ y_\xi(\xi_i,\eta_j) \\ y_\eta(\xi_i,\eta_j) \\ y_{\xi\eta}(\xi_i,\eta_j) \end{bmatrix} \qquad Y_3^{(i,j)} = \begin{bmatrix} y(\xi_i,\eta_{j+1}) \\ y_\xi(\xi_i,\eta_{j+1}) \\ y_\eta(\xi_i,\eta_{j+1}) \\ y_{\xi\eta}(\xi_i,\eta_{j+1}) \end{bmatrix}$$

$$Y_2^{(i,j)} = \begin{bmatrix} y(\xi_{i+1},\eta_j) \\ y_\xi(\xi_{i+1},\eta_j) \\ y_\eta(\xi_{i+1},\eta_j) \\ y_{\xi\eta}(\xi_{i+1},\eta_j) \end{bmatrix} \qquad Y_4^{(i,j)} = \begin{bmatrix} y(\xi_{i+1},\eta_{j+1}) \\ y_\xi(\xi_{i+1},\eta_{j+1}) \\ y_\eta(\xi_{i+1},\eta_{j+1}) \\ y_{\xi\eta}(\xi_{i+1},\eta_{j+1}) \end{bmatrix} \tag{60}$$

If we increase the row index from i to i+1, then the grid point shifts down by one step and the following holds

$$Y_1^{(i+1,j)} = Y_2^{(i,j)} \qquad Y_3^{(i+1,j)} = Y_4^{(i,j)} \tag{61}$$

If we increase the column index from j to j+1 then the grid point shifts to the right by one step and one obtains

$$Y_1^{(i,j+1)} = Y_3^{(i,j)} \qquad Y_2^{(i,j+1)} = Y_4^{(i,j)} \tag{62}$$

The following diagram shows the relationship of the grid system.

$$
\begin{array}{ccccccc}
 & & & \vdots & & & \\
Y_1^{(i,j)} & & Y_3^{(i,j)} & = & Y_1^{(i,j+1)} & & Y_3^{(i,j+1)} \\
 & [Y^{(i,j)}] & & & & [Y^{(i,j+1)}] & \\
Y_2^{(i,j)} & & Y_4^{(i,j)} & = & Y_2^{(i,j+1)} & & Y_4^{(i,j+1)} \\
\cdots \; \| & & \| & & \| & & \| \; \cdots \\
Y_1^{(i+1,j)} & & Y_3^{(i+1,j)} & = & Y_1^{(i+1,j+1)} & & Y_3^{(i+1,j+1)} \\
 & [Y^{(i+1,j)}] & & & & [Y^{(i+1,j+1)}] & \\
Y_2^{(i+1,j)} & & Y_4^{(i+1,j)} & = & Y_2^{(i+1,j+1)} & & Y_4^{(i+1,j+1)} \\
 & & & \vdots & & &
\end{array}
$$

SPLINE FUNCTION

We may express the variables $y^{(i,j)}$ and $\delta y^{(i,j)}$ in Eq. (58) in terms of the (1x16) spline function $a^T(\xi,\eta)$ and the (16x1) node point function $Y^{(i,j)}$ as follows.

$$y^{(i,j)}(\xi,\eta) = a^T(\xi,\eta)Y^{(i,j)} \tag{63}$$

where

$$a^T(\xi,\eta) = \{[a^1(\xi,\eta)]^T \; [a^2(\xi,\eta)]^T \; [a^3(\xi,\eta)]^T \; [a^4(\xi,\eta)]^T \tag{64}$$

and

$$\delta\bar{y}^{(i,j)}(\xi,\eta) = a^T(\xi,\eta)\delta\bar{Y}^{(i,j)} \tag{65}$$

A typical term for a product can be written as

$$\delta\bar{y}^{(i,j)}y^{(i,j)} = [\delta\bar{Y}^{(i,j)}]^T a(\xi,\eta)a^T(\xi,\eta)Y^{(i,j)} \tag{66}$$

BICUBIC HERMITE POLYNOMIAL SPLINES

With the aid of Eq. (59), Eq. (63) may be expressed as

$$y^{(i,j)}(\xi,\eta) = [a^1(\xi,\eta)]^T Y_1^{(i,j)} + [a^2(\xi,\eta)]^T Y_2^{(i,j)} + [a^3(\xi,\eta)]^T Y_3^{(i,j)} + [a^4(\xi,\eta)]^T Y_4^{(i,j)} \tag{67}$$

The bicubic Hermite polynomial spline is continuous in the functional value, its first partials in two directions, and its mixed first partial in both directions. The bicubic Hermite polynomial spline gives

$$a^1(\xi,\eta) = \begin{bmatrix} \phi(\xi)\ \phi(\eta) \\ \psi[\xi)\ \phi(\eta) \\ \phi(\xi)\ \psi(\eta) \\ \psi(\xi)\ \psi(\eta) \end{bmatrix}^T \qquad a^3(\xi,\eta) = \begin{bmatrix} \phi(\xi)\ \rho(\eta) \\ \psi(\xi)\ \rho(\eta) \\ \phi(\xi)\ \omega(\eta) \\ \psi(\xi)\ \omega(\eta) \end{bmatrix}^T$$

$$a^2(\xi,\eta) = \begin{bmatrix} \rho(\xi)\ \phi(\eta) \\ \omega(\xi)\ \phi(\eta) \\ \rho(\xi)\ \psi(\eta) \\ \omega(\xi)\ \psi(\eta) \end{bmatrix}^T \qquad a^4(\xi,\eta) = \begin{bmatrix} \rho(\xi)\ \rho(\eta) \\ \omega(\xi)\ \rho(\eta) \\ \rho(\xi)\ \omega(\eta) \\ \omega(\xi)\ \omega(\eta) \end{bmatrix}^T \tag{68}$$

where

$$\begin{aligned} \phi(\xi) &= 1 - 3\xi^2 + 2\xi^3 & \phi_\xi(\xi) &= -6\xi + 6\xi^2 \\ \psi(\xi) &= \xi - 2\xi^2 + \xi^3 & \psi_\xi(\xi) &= 1 - 4\xi + 3\xi^2 \\ \rho(\xi) &= 3\xi^2 - 2\xi^3 & \rho_\xi(\xi) &= 6\xi - 6\xi^2 \\ \omega(\xi) &= -\xi^2 + \xi^3 & \omega_\xi(\xi) &= -2\xi + 3\xi^2 \end{aligned} \tag{69}$$

At grid points (nodes) the value of ξ or η takes the value of 0 or 1. Thus we have

$$\begin{bmatrix} \phi(0) = 1 & \psi(0) = 0 & \phi(1) = 0 & \psi(1) = 0 \\ \phi_\xi(0) = 0 & \psi_\xi(0) = 1 & \phi_\xi(1) = 0 & \psi_\xi(1) = 0 \\ \rho(0) = 0 & \omega(0) = 0 & \rho(1) = 1 & \omega(1) = 0 \\ \rho_\xi(0) = 0 & \omega_\xi(0) = 0 & \rho_\xi(1) = 0 & \omega_\xi(1) = 1 \end{bmatrix} \tag{70}$$

It is noted that the diagonal elements of the matrix are unity and the off diagonal terms are zeroes. Similar expressions are held for $\phi(\eta)$, etc. in terms of η. For example

$$\phi(\eta) = 1 - 3\eta^2 + 2\eta^3 \text{ , etc.} \tag{71}$$

CONSISTENCY AT NODES

To show that Eqs. (67) through (69) are consistent at the node points, we will check only the following cases.

(1) For the case $\xi = 0$ and $\eta = 0$, from Eqs. (68) and (70) we have

$$a^2(0,0) = a^3(0,0) = a^4(0,0) = [0\ 0\ 0\ 0]$$
$$a^1(0,0) = [1\ 0\ 0\ 0] \tag{72}$$

(a)
$$y^{(i,j)}(\xi,\eta)\Big|_{\substack{\xi=0\\ \eta=0}} = [a^1(\xi,\eta)]^T_{\substack{\xi=0\\ \eta=0}} Y_1^{(i,j)}$$
$$= [1\ 0\ 0\ 0]Y_1^{(i,j)} = y^{(i,j)}(0,0) \tag{73}$$

(b) $$y_\xi^{(i,j)}(\xi,\eta)\Big|_{\substack{\xi=0\\ \eta=0}} = [a^1{}_\xi(\xi,\eta)]^T{}_{\substack{\xi=0\\ \eta=0}} Y_1^{(i,j)}$$

$$= \begin{bmatrix} \phi_\xi(\xi)\ \phi(\eta) \\ \psi_\xi(\xi)\ \phi(\eta) \\ \phi_\xi(\xi)\ \psi(\eta) \\ \psi_\xi(\xi)\ \psi(\eta) \end{bmatrix}^T_{\substack{\xi=0\\ \eta=0}} \begin{bmatrix} y^{(i,j)}(0,0) \\ y_\xi^{(i,j)}(0,0) \\ y_\eta^{(i,j)}(0,0) \\ y_{\xi\eta}^{(i,j)}(0,0) \end{bmatrix}$$

$$= [0\ 1\ 0\ 0]Y_1^{(i,j)}$$

$$= y_\xi^{(i,j)}(0,0) \tag{74}$$

(c) $$y_{\xi\eta}^{(i,j)}(\xi,\eta)\Big|_{\substack{\xi=0\\ \eta=0}} = [a^1{}_{\xi\eta}(\xi,\eta)]^T{}_{\substack{\xi=0\\ \eta=0}} Y_1^{(i,j)}$$

$$= \begin{bmatrix} \phi_\xi(\xi)\ \phi_\eta(\eta) \\ \psi_\xi(\xi)\ \phi_\eta(\eta) \\ \phi_\xi(\xi)\ \psi_\eta(\eta) \\ \psi_\xi(\xi)\ \psi_\eta(\eta) \end{bmatrix}^T_{\substack{\xi=0\\ \eta=0}} \begin{bmatrix} y^{(i,j)}(0,0) \\ y_\xi^{(i,j)}(0,0) \\ y_\eta^{(i,j)}(0,0) \\ y_{\xi\eta}(i,j)(0,0) \end{bmatrix}$$

$$= [0\ 0\ 0\ 1]Y_1^{(i,j)}$$

$$= y_{\xi\eta}^{(i,j)}(0,0) \tag{75}$$

The above expressions show that the function, its first partial in one direction, and its mixed partial are consistent and continuous at the node point $\xi = 0$ and $\eta = 0$.

(2) For the case $\xi = 1$ and $\eta = 1$, from Eqs. (68) and (70) we have

$$a^1(1,1) = a^2(1,1) = a^3(1,1) = [0\ 0\ 0\ 0]$$

$$a^4(1,1) = [1\ 0\ 0\ 0] \tag{76}$$

(a) Thus

$$y^{(i,j)}(\xi,\eta)\Big|_{\substack{\xi=1\\ \eta=1}} = [a^4(\xi,\eta)]^T_{\substack{\xi=1\\ \eta=1}}\ Y_4^{(i,j)}$$

$$= [1\ 0\ 0\ 0]Y_4^{(i,j)} = y^{(i,j)}(1,1) \tag{77}$$

(b)

$$y_\xi^{(i,j)}(\xi,\eta)\Big|_{\substack{\xi=1\\ \eta=1}} = [a^4{}_\xi(\xi,\eta)]^T_{\substack{\xi=1\\ \eta=1}}\ Y_4^{(i,j)}$$

$$= \begin{bmatrix} \rho_\xi(\xi)\ \rho(\eta) \\ \omega_\xi(\xi)\ \rho(\eta) \\ \rho_\xi(\xi)\ \omega(\eta) \\ \omega_\xi(\xi)\ \omega(\xi) \end{bmatrix}^T_{\substack{\xi=1\\ \eta=1}} \begin{bmatrix} y^{(i,j)}(1,1) \\ y_\xi^{(i,j)}(1,1) \\ y_\eta^{(i,j)}(1,1) \\ y_{\xi\eta}(i,j)(1,1) \end{bmatrix}$$

$$= [0\ 1\ 0\ 0]Y_4^{(i,j)} = y_\xi^{(i,j)}(1,1) \tag{78}$$

(c)

$$y_{\xi\eta}^{(i,j)}(\xi,\eta)\Big|_{\substack{\xi=1\\ \eta=1}} = [a^4{}_{\xi\eta}(\xi,\eta)]^T_{\substack{\xi=1\\ \eta=1}}\ Y_4^{(i,j)}$$

$$= \begin{bmatrix} \rho_\xi(\xi)\ \rho_\eta(\eta) \\ \omega_\xi(\xi)\ \rho_\eta(\eta) \\ \rho_\xi(\xi)\ \omega_\eta(\eta) \\ \omega_\xi(\xi)\ \omega_\eta(\eta) \end{bmatrix}^T_{\substack{\xi=1\\ \eta=1}} \begin{bmatrix} y^{(i,j)}(1,1) \\ y_\xi^{(i,j)}(1,1) \\ y_\eta^{(i,j)}(1,1) \\ y_{\xi\eta}^{(i,j)}(1,1) \end{bmatrix}$$

$$= [0\ 0\ 0\ 1]Y_4^{(i,j)} = y_{\xi\eta}^{(i,j)}(1,1) \tag{79}$$

It can be proved that all the 16 elements at four corners of the grid are consistent. It can also be proved that the function, its two directional first derivatives and its mixed partial are continuous at all grid points.

WAVE EQUATION

Let us take a special care for further study of the mixed initial and boundary value problems. We choose the wave equation where the parameters in Eq. (24) are

$$\beta = \gamma = \mu = \nu = \varepsilon = 0 \tag{80}$$

$$\text{and } \alpha = \text{const} \neq 0 \tag{81}$$

$$\ell = \text{const} \neq 0 \tag{82}$$

Then Eq. (24) becomes

$$Ly = \alpha y_{tt} + \ell y_{xx} = -Q \tag{83}$$

Eq. (58) is simplified to

$$\begin{aligned}
\delta J(\delta\bar{y}) = {} & \sum_{j=1}^{K} \frac{\alpha H}{K} \int_0^1 \delta\bar{y}(i,j) y_\xi(i,j) d\eta \Big|_{t_o}^{t_b} \\
& + \sum_{i=1}^{H} \frac{\ell K}{H} \int_0^1 \delta\bar{y}(i,j) y_\eta(i,j) d\xi \Big|_{x_o}^{x_b} \\
& + \sum_{j=1}^{K} \sum_{i=1}^{H} \frac{1}{HK} \int_0^1 \int_0^1 \delta\bar{y}(i,j) Q d\xi d\eta \\
& + \sum_{j=1}^{K} \sum_{i=1}^{H} \int_0^1 \int_0^1 [\frac{\alpha H}{K} \delta\bar{y}_\xi(i,j) y_\xi(i,j) \\
& + \frac{\ell K}{H} \delta\bar{y}_\eta(i,j) y_\eta(i,j)] d\xi d\eta = 0
\end{aligned} \tag{84}$$

Differentiating Eqs. (63) and (65), and substituting into Eq. (84) we have

$$\delta J(\delta\bar{y}) = \sum_{j=1}^{K} \frac{\alpha H}{K} [\delta\bar{Y}(i,j)]^T \int_0^1 a(\xi,\eta) a_\xi(\xi,\eta) d\eta \Big|_{t_o}^{t_b} Y(i,j)$$

$$+ \sum_{i=1}^{H} \frac{\ell K}{H} [\delta\bar{Y}(i,j)]^T \int_0^1 a(\xi,\eta) a_\eta(\xi,\eta) d\xi \Big|_{x_o}^{x_b} Y(i,j)$$

$$+ \sum_{j=1}^{K} \sum_{i=1}^{H} \frac{1}{HK} [\delta\bar{Y}(i,j)]^T \int_0^1 \int_0^1 a(\xi,\eta) Q(\xi,\eta) d\xi d\eta$$

$$+ \sum_{j=1}^{K} \sum_{i=1}^{H} \frac{\alpha H}{H} [\delta\bar{Y}(i,j)]^T \int_0^1 \int_0^1 a_\xi(\xi,\eta) a_\xi^T(\xi,\eta) d\xi d\eta \, Y(i,j)$$

$$+ \sum_{j=1}^{K} \sum_{i=1}^{H} \frac{\ell K}{H} [\delta\bar{Y}(i,j)]^T \int_0^1 \int_0^1 a_\eta(\xi,\eta) a_\eta^T(\xi,\eta) d\xi d\eta \, Y(i,j) = 0 \quad (85)$$

Eq. (85) may be written into a different form as

$$\delta J(\delta\bar{y}) = \sum_{j=1}^{K} [\delta\bar{Y}(t_b,j)]^T P_{0\xi}(t_b) Y(t_b,j)$$

$$- \sum_{j=1}^{K} [\delta\bar{Y}(t_o,j)]^T P_{0\xi}(t_o) Y(t_o,j)$$

$$+ \sum_{i=1}^{H} [\delta\bar{Y}(i,x_b)]^T P_{0\eta}(x_b) Y(i,x_b)$$

$$- \sum_{i=1}^{H} [\delta\bar{Y}(i,x_o)]^T P_{0\eta}(x_o) Y(i,x_o)$$

$$+ \sum_{j=1}^{K} \sum_{i=1}^{H} [\delta\bar{Y}(i,j)]^T q(i,j)$$

$$- \sum_{j=1}^{K} \sum_{i=1}^{H} [\delta\bar{Y}(i,j)]^T p(i,j) Y(i,j) = 0 \quad (86)$$

It is noted that the first two terms involve initial values, the next two terms involve boundary values, and the last two terms involve interior quantities within the region.

Equation (86) uses the following notations

$$P_{0\xi}(t_b) = \frac{\alpha H}{K} \int_0^1 a(\xi,\eta)a_\xi^T(\xi,\eta)d\eta \Big|_{t=t_b} \tag{87}$$

$$P_{0\xi}(t_o) = \frac{\alpha H}{K} \int_0^1 a(\xi,\eta)a_\xi^T(\xi,\eta)d\eta \Big|_{t=t_o} \tag{88}$$

$$P_{0\eta}(x_b) = \frac{\ell K}{K} \int_0^1 a(\xi,\eta)a_\eta^T(\xi,\eta)d\xi \Big|_{x=x_b} \tag{89}$$

$$P_{0\eta}(x_o) = \frac{\ell K}{K} \int_0^1 a(\xi,\eta)a_\eta^T(\xi,\eta)d\xi \Big|_{x=x_o} \tag{90}$$

$$P = \frac{\alpha H}{K} P_{\xi\xi} + \frac{\ell K}{H} P_{\eta\eta} \tag{91}$$

$$P_{\xi\xi} = \int_0^1 \int_0^1 a_\xi(\xi,\eta)a_\xi^T(\xi,\eta)d\xi d\eta \tag{92}$$

$$P_{\eta\eta} = \int_0^1 \int_0^1 a_\eta(\xi,\eta)a_\eta^T(\xi,\eta)d\xi d\eta \tag{93}$$

and

$$q(i,j) = \frac{1}{HK} \int_0^1 \int_0^1 a(\xi,\eta)Q(\xi,\eta)d\xi d\eta \tag{94}$$

For a given spline function, such as bicubic Hermite polynomials, $a(\xi,\eta)$ is given in Eqs. (64), (68), and (69). For a given grid the number of node points are known, so are H and K. Thus Eqs. (87) through (93) can be determined and stored in advance. For any given forcing function $Q(\xi,\eta)$, Eq. (94) can also be evaluated.

The (16x1) vector $Y^{(i,j)}$ in Eq. (86) was defined in Eq. (59). Its components can be overlapped as given in Eqs. (61) and (62). We have found previously that the first term in Eq. (86) can be dropped because it can automatically satisfy the final conditions for an initial value problem. In the second term the function $Y^{(t_o,j)}$ is known because the coefficients are the initial values. Although some of the boundary values $Y^{(i,x_b)}$ amd $Y^{(i,x_o)}$ are given, most of these terms are to be determined. The entire problem is to solve for $Y^{(i,j)}$ by setting to zero the assembly coefficients of the individual elements of $\delta Y^{(i,j)}$.

It is a tedious task to assemble these coefficients. These will be performed in the future as a separate report.

CONCLUSION

A bilinear form of the original and adjoint variable is employed in determining the coefficients of the variations of the functions and their first derivatives. There is no term involving the variations of any higher derivatives. A bicubic Hermite polynomial is used which gives continuity in the functions and first partial derivatives in space <u>or</u> time, together with the mixed first partial derivative in space <u>and</u> time. In solving mixed boundary and initial value problems of a second order partial differential equation using spline functions, the computation may be simplified considerably if the variable in time can be truncated into arbitrary sections. The entire problem is divided into several strips of distinct time intervals, each strip containing mostly the boundary value problem.

The variational principle for spatial and temporal problems with boundary and initial conditions has been investigated. This variational principle is very general in scope and can be applied to many linear partial differential equations. The principle is applicable if the bilinear concomitant is identically zero. This leads to the requirement that a set of end conditions for the adjoint systems must be found to satisfy this condition. Otherwise the variational principle as stated may not be applicable.

Both the wave equation and the heat equation (with one dimensional spatial direction) satisfy these variational principles. For future work the analytic solution of these equations using the finite element method will be studied. The assembly of the elements of the matrices involved in the formulation will be demonstrated. The stability problem in numerical solutions on these equations will also be investigated. This lays the foundation for the gun dynamics problem to be studied in the future.

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